Systematic comparison of position and time dependent macroparticle simulations in beam dynamics studies

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Macroparticle simulation plays an important role in modern accelerator design and operation. Most linear rf accelerators have been designed based on macroparticle simulations using longitudinal position as the independent variable. In this paper, we have done a systematic comparison between using longitudinal position as the independent variable and using time as the independent variable in macroparticle simulations. We have found that, for an rms-matched beam, the maximum relative moment difference for second, fourth moments and beam maximum amplitudes between these two types of simulations is 0.25% in a 10 m reference transport system with physical parameters similar to the Spallation Neutron Source linac design. The maximum z-to-t transform error in the space-charge force calculation of the position dependent simulation is about 0.1% in such a system. This might cause a several percent error in a complete simulation of a linac with a length of hundreds of meters. Furthermore, the error may be several times larger in simulations of mismatched beams. However, if such errors are acceptable to the linac designer, then one is justified in using position dependent macroparticle simulations in this type of linac design application.

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I. INTRODUCTION

Macroparticle simulation plays an invaluable role in modern accelerator design. It provides a quantitative prediction of the dynamics of a bunch of charged particles in the accelerator. The charged particles in the bunch are subject to the external focusing and accelerating forces and also to the space-charge forces from intraparticle Coulomb interactions within the bunch. With increasing interest in utilizing high-intensity beams for future accelerator applications, e.g., accelerator-driven spallation neutron production for basic and applied research, the accelerator production of tritium, and the accelerator transmutation of radioactive waste, an accurate treatment of space-charge forces becomes more important in accelerator design and operation. A self-consistent method of describing high-intensity beams subject to external fields and space-charge forces is to solve the Poisson-Vlasov equation. The most widely used method in accelerator physics for solving the Poisson-Vlasov equation is to use macroparticle simulations based on the particle-in-cell (PIC) method [1–8].

The PIC approach to modeling charged-particle beams generally uses one of two possible independent variables: the time, t, or the arc length, s (the latter corresponding to the longitudinal coordinate, z, in the case of a linac whose reference trajectory coincides with the z axis). The space-charge forces are most naturally handled using a time-based code, since the self-fields are based on the solution of Poisson's equation at *fixed time*. However, it is challenging to simulate beam dynamics in a time-based code when the external fields are specified as piecewise constant functions of position. This has led, for example, to the use of "residence correction algorithms" in time-based codes used by the heavy ion fusion community, when integrating the trajectories of particles as they cross from one beam line element to the next [3]. This ceases to be an issue when realistic fringe fields (rather than hard-edged fields) are used in the computer models, or when the potentials are specified in terms of z-dependent smoothly varying functions as is the case with RFQs. However, the use of a time-based approach is still a departure from the approach that is virtually always used for the zero-current beam optics design (particularly for studying nonlinear effects and for designing circular systems), namely, the use of map-based techniques for which s or z is the independent variable.

In contrast, using z as the independent variable has the advantage of allowing a simpler treatment of the external fields. Additionally, we can calculate the transfer maps corresponding to the external field and advance the particles using these transfer maps and the space-charge forces using a split-operator method [7]. This can significantly improve the computation speed compared to a step-by-step integration through the external field. However, in the z-dependent simulation, the space-charge forces need to be computed at a fixed time. The particle distribution at a given z location has to be transformed back into a distribution at a fixed time before the calculation of the space-charge forces can be completed. In the usual approach, this transformation is achieved by following a straight line back to the fixed time. Such a transformation neglects the acceleration of the particles and the time and position variation of the external and space-charge forces during the transformation. Nevertheless, given the typical parameters in a high-intensity rf linac (bunch length, energy spread, momentum spread, etc.), the instantaneous error in the transformation may be very small — the accuracy of the approximation depends only on the deviation of the trajectories from straight lines over a time interval corresponding to the spread in arrival times of particles within a bunch. However, the cumulative effect of this error may be a cause for concern (as will be shown below).

In a previous study, Jameson compared a position-based code and a time-based code for modeling beam dynamics in an RFQ [9]. The study concluded that the time-based code should be used since the position-based code tended to underestimate the fraction of the lost beam through the RFQ, and produced significant errors in the beam loss pattern. In this case, the input dc beam has a large phase and energy spread, hence the errors in the z-to-t transformation in the space-charge calculation of a position-based code would be significant. However, for a bunched beam with small phase and energy spread, this transformation error may be tolerable. For example, the widely used linac design code, PARMILA, uses position as the independent variable in the beam dynamics simulation beyond the RFQ, for structures such as a drift-tube linac (DTL), a coupled-cavity linac, and a superconducting linac [5]. To the best of our knowledge, no systematic study has been done previously to compare the results of the t-based and z-based approaches in these structures. Preliminary benchmarking of different codes for the first tank of the Spallation Neutron Source (SNS) DTL all gave similar results [10]. A systematic comparison will help to establish the valid regimes for use of the z-to-t transformation and to verify our confidence in the use of position dependent codes such as PARMILA for accelerator design. In this paper, we present the results of a systematic comparison of these two types of simulations using a reference transport system with physical parameters similar to the SNS linac. The choice of an independent variable affects the accuracy of the simulation with regard to the calculation of the space-charge forces and hence the accuracy of the particle trajectories. This leads to changes in the prediction of the evolution of the beam distribution, both in the core and in the halo. For this reason, we have chosen three criteria to compare the two types of simulations (position dependent and time dependent). One criterion is the second moment, which provides information about the beam core; another criterion is the fourth moment, which is more strongly affected by the tail of the distribution than the second moment. A third criterion is the maximum particle amplitude, i.e., the amplitude of the outermost particle in the simulation. This is especially important, because it affects the prediction of the location at which particles are lost, and because uncertainty in that prediction also affects the energy of the lost particles. Whenever the maximum particle amplitude is greater than the accelerator aperture or the rf bucket size, a particle is lost, and this may lead to radioactivation of accelerator components.

II. COMPUTATIONAL MODELS

The charged particles moving in an accelerator can be described by the Poisson-Vlasov equation:

$$\frac{\partial f}{\partial t} + \dot{\mathbf{r}} \cdot \frac{\partial f}{\partial \mathbf{r}} + \dot{\mathbf{p}} \cdot \frac{\partial f}{\partial \mathbf{p}} = 0\,, \tag{1}$$

where f denotes the distribution function of the particles, and where a dot denotes the derivative with respect to time. The quantity $\mathbf{r}$ is the spatial position and $\mathbf{p}$ is the mechanical momentum which satisfies $\dot{\mathbf{p}} = \mathbf{F}$. The force $\mathbf{F}$ includes the contributions from both the externally applied fields and the space-charge fields. The space-charge fields are treated in a mean-field approximation to the N-body microparticle Coulomb field. In the moving frame, the space-charge force, $\mathbf{F}_{\mathrm{sc}}$ can be obtained from the solution of Poisson's equation

$$\nabla^2 \phi(\mathbf{r}) = -\frac{\rho(\mathbf{r})}{\epsilon_0}\,, \tag{2}$$

and

$$\mathbf{F}_{\mathrm{sc}} = -q\nabla\phi\,, \tag{3}$$

where ϕ is the electrostatic potential in the moving frame, ρ is the particle spatial charge density, and ϵ_0 is the vacuum permittivity. The charge density can be calculated from the distribution function, f, by

$$\rho(\mathbf{r}) = \int d^3\mathbf{p}\, f(\mathbf{r}, \mathbf{p})\,. \tag{4}$$

The solution of Poisson's equation can be written as

$$\phi(\mathbf{r}) = \int G(\mathbf{r}, \mathbf{r}')\rho(\mathbf{r}')\, d\mathbf{r}'\,, \tag{5}$$

where G is the Green's function. For the case of three-dimensional open boundary conditions, the Green's function can be written as

$$G(\mathbf{r}, \mathbf{r}') = \frac{1}{4\pi\epsilon_0|\mathbf{r} - \mathbf{r}'|}\,. \tag{6}$$

The Poisson-Vlasov equation can be modeled using the particle-in-cell approach. Here, macroparticles are generated with the same charge-to-mass ratio as the real particles in the bunch. The equations of motion using t as the independent variable are

$$\dot{x} = \frac{p_x c}{\gamma}\,, \tag{7}$$

$$\dot{y} = \frac{p_y c}{\gamma}\,, \tag{8}$$

$$\dot{z} = \frac{p_z c}{\gamma}\,, \tag{9}$$

$$\dot{p}_x = \frac{q}{m_0 c}\left(\mathbf{E} + \frac{c}{\gamma}\mathbf{p} \times \mathbf{B}\right)_x, \tag{10}$$

$$\dot{p}_y = \frac{q}{m_0 c}\left(\mathbf{E} + \frac{c}{\gamma}\mathbf{p} \times \mathbf{B}\right)_y, \tag{11}$$

$$\dot{p}_z = \frac{q}{m_0 c}\left(\mathbf{E} + \frac{c}{\gamma}\mathbf{p} \times \mathbf{B}\right)_z, \tag{12}$$

where $p_x = \gamma\beta_x$, $p_y = \gamma\beta_y$, $p_z = \gamma\beta_z$, $\gamma = 1/\sqrt{1-\beta^2}$, $\beta_i = \frac{v_i}{c}$ with $i = x, y, z$; c is the speed of light, and m_0 is the rest mass of the particle. The electric field, $\mathbf{E}$, and magnetic field, $\mathbf{B}$, include the contributions from external focusing and accelerating fields and the mean field of the intraparticle Coulomb interactions.

Using z as the independent variable, the equations of motion are

$$x' = \frac{p_x}{p_z}, \tag{13}$$

$$y' = \frac{p_y}{p_z}, \tag{14}$$

$$\psi' = \frac{\frac{\omega}{c}\gamma}{p_z} - \frac{\frac{\omega}{c}}{\beta_0}, \tag{15}$$

$$p_x' = \frac{q}{m_0 c p_z}\left(\frac{\gamma}{c}\mathbf{E} + \mathbf{p} \times \mathbf{B}\right)_x, \tag{16}$$

$$p_y' = \frac{q}{m_0 c p_z}\left(\frac{\gamma}{c}\mathbf{E} + \mathbf{p} \times \mathbf{B}\right)_y, \tag{17}$$

$$p_t' = \frac{q}{m_0 c^2} E_{z0} - \frac{q}{m_0 c^2 p_z}\mathbf{p} \cdot \mathbf{E}, \tag{18}$$

where ψ is the phase relative to the reference particle defined by $\psi = \omega(t - t_g)$, ω is the assumed rf frequency, t_g is the flight time of the reference particle, p_t is the normalized energy deviation with respect to the reference particle, and $p_t = \gamma_g - \gamma$, where γ_g is the γ of the reference particle. The trajectory of the reference particle on the axis of the accelerator can be determined from the following:

$$t_g' = \frac{1}{\beta_0 c}, \tag{19}$$

$$\gamma_g' = \frac{q}{m_0 c^2} E_{z0}(z, t), \tag{20}$$

where E_{z0} is the on-axis external electric field (with the on-axis space-charge field assumed to be zero at the location of the reference particle), and $\beta_0 = \sqrt{1 - 1/\gamma_g^2}$.

In our simulations, for both methods, the equations of motion for the macroparticles are integrated using a second-order leapfrog algorithm. Within each step, the particle coordinates are advanced in space by a half step using their present velocities. Then the particles are deposited onto a three-dimensional spatial grid to obtain the charge density distribution. In the case of using z as the independent variable, the particles at a given longitudinal position need to be transformed back to the distribution at a fixed time before deposition to the grid. Two types of transformations have been used in the literature [5,7]. In the first transformation, the momentum and energy spread in the beam bunch are assumed to be small and negligible. This transformation has the form

$$x^t = x^z, \tag{21}$$

$$y^t = y^z, \tag{22}$$

$$\delta z = -\frac{c}{\omega}\beta_0\psi, \tag{23}$$

where δz is the particle longitudinal distance with respect to the reference particle in the laboratory frame. This transformation is the simplest (and crudest) possible, since it does not take into account the relative change of the transverse location of particles and it neglects how the different energies of the particles affect their longitudinal positions. We prefer a second transformation, which assumes that all particles move ballistically within the maximum phase deviation of the beam bunch. This transformation has the form

$$x^t = x^z - \frac{c}{\omega} p_x\psi/\gamma, \tag{24}$$

$$y^t = y^z - \frac{c}{\omega} p_y\psi/\gamma, \tag{25}$$

$$\delta z = -\frac{c}{\omega}\beta_z\psi. \tag{26}$$

This transformation is superior to the one mentioned previously, since it includes the effects of momentum and energy spread in the beam. Note, however, that the presence of the external fields and the space-charge fields during the transformation are both neglected.

Having obtained the charge density at a fixed time, the remainder of the calculation proceeds as follows: The charge density is accumulated on a grid using an area weighting scheme, and the convolution given by Eq. (5) is calculated using a fast-Fourier transform-based algorithm [11]. The electric fields on the grid are calculated from the potential using a central finite-difference scheme. The fields on the grid are reinterpolated back to the particles to obtain the total space-charge force on the particles. The momenta of the particles are then advanced by one step using both the external fields and the space-charge forces.

Finally, the particles are advanced another half step using the updated velocities to complete a full step.

III. SYSTEMATIC COMPARISON

The macroparticle simulation using time as the independent variable has been assumed as the baseline result in the comparison. In order to verify that the space-charge forces have been correctly calculated in the time dependent simulation, we simulated a case that can be solved analytically. Two charged particles of identical mass and opposite charge are initially placed at the two opposite diagonal corners of a cubic box. The initial speed of the two particles is given by

$$|v| = \sqrt{\frac{q^2}{4\pi\epsilon_0 m_0 r}}, \tag{27}$$

where r is the distance from the corner of the box to the center of the box. If the calculation of the space-charge forces has been done correctly, the two particles will rotate around the center of the box with a fixed radius r. Figure 1 shows, for the two particles, the rms value of position and radius as a function of time. As expected, the radius is independent of time since we chose the center of the orbits to be at the origin.

In order to systematically compare the macroparticle simulations using time, t, and position, z, as independent variables, we have set up a periodic transport system with a total length of about 10 m. Each period contains a FODO [sequence focusing, drift gap (zero focusing), defocusing, drift gap element array] quadrupole focusing channel with two rf gaps between them to provide acceleration and longitudinal focusing. The quadrupole length is 8 cm with a focusing gradient of 26 T/m. The fields in the rf gap have sinusoidal longitudinal position dependence and are given by

$$e(z) = e_0 \sin(8\pi z/L), \tag{28}$$

$$E_x = -xe'(z)\cos(\omega t + \theta_0)/2, \tag{29}$$

$$E_y = -ye'(z)\cos(\omega t + \theta_0)/2, \tag{30}$$

$$E_z = -\left\{e(z) - \frac{r^2}{4}\left[e''(z) + \frac{\omega^2}{c^2}e(z)\right]\right\}\cos(\omega t + \theta_0), \tag{31}$$

$$B_x = y\frac{\omega}{c^2}e(z)\sin(\omega t + \theta_0)/2, \tag{32}$$

$$B_y = -x\frac{\omega}{c^2}e(z)\sin(\omega t + \theta_0)/2, \tag{33}$$

$$B_z = 0.0, \tag{34}$$

where the superscript prime is the derivative with respect to z, L is the length of the rf cavity, ω is the frequency of the rf field, θ_0 is the drive phase, and e_0 is the amplitude of the rf field which is 8 MV/m in the reference case. The zero-current transverse and longitudinal phase advances through one period are 78° and 60°, respectively. The reference current used here is 112 mA, which results in a 0.57 transverse rms tune depression and a 0.46 longitudinal rms tune depression. The whole transport system consists of five periods. The initial kinetic energy is 88 MeV and the final kinetic energy is 98 MeV. The physical parameters used here are chosen to maintain similarity to the present SNS linac design. These parameters form a reference case in the following study.

The initial particle distribution is generated as a Waterbag distribution having rms sizes satisfying the matched-beam conditions in the first period of the transport system. Figure 2 shows the rms size of the distribution of particles moving through the reference case transport system. It appears that the beam is well matched transversely. The longitudinal rms bunch length grows from 1.3 to 1.7 mm through the system. The effect of the increasing bunch length is of particular interest since the longer bunch length will generally degrade the accuracy of

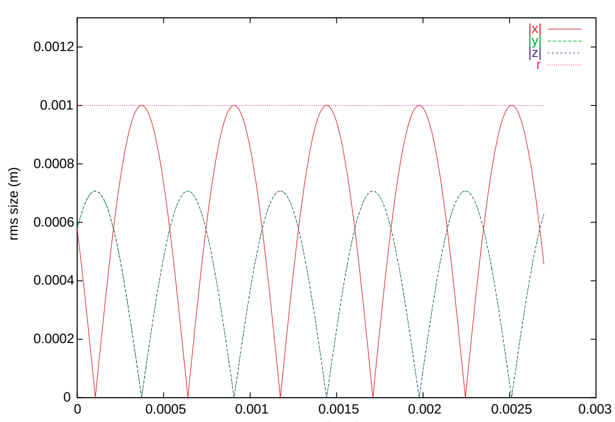

FIG. 1. (Color) The position and radius of the rotating particle as a function of time.

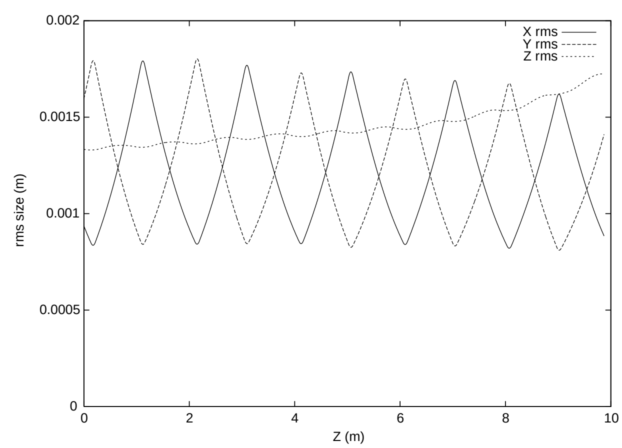

FIG. 2. The rms size of the particles for the reference transport system.

the z-to-t transformation for the space-charge force calculation in a z-dependent simulation.

Figure 3 shows the relative differences between the z-dependent macroparticle simulation (z code) and the t-dependent simulation (t code) in this reference case. In the figure, the relative difference δM is defined as

$$\delta M = \frac{|M^z - M^t|}{M^t}, \tag{35}$$

where M^z is the moment of the distribution calculated from the z code, and M^t is the moment from the t code. The relative differences of the second moments, the fourth moments, and the maximum amplitudes of the particles are calculated as a function of z and are shown in the figure. In order to make a direct comparison, we have also transformed the particle distribution from given z to a fixed t in the z-dependent simulation before computing the moments.

It is seen from Fig. 3 that the maximum relative difference after 10 m is only 0.25%. As discussed earlier, we have used the first-order transformation before the calculation of space-charge forces in the z code since this transformation is believed to be more accurate than the zeroth-order transformation. The differences observed in Fig. 3 could be caused by a number of computational errors associated with the macroparticle simulation. There are computational errors from the finite number of particles used, finite grid size in the numerical solution of Poisson's equation on the grid, finite integration step size, and the z-to-t transformation error in the z-dependent simulation. The first three types of errors are controllable errors which can be systematically reduced using more macroparticles, finer grid size, and smaller step size. The z-to-t transformation error in the z-dependent simulation contributes to an error in the calculation of the space-charge force and cannot be reduced by changing the simulation parameters except by using a more complicated transformation algorithm or an alternate approach that uses multiple reference particles to shorten the interval over which the transformation is applied. We call this error an uncontrollable error.

The size of the z-to-t transformation error can be estimated by comparing the results of Fig. 3 with analogous results produced by performing the simulation with zero current. This is shown in Fig. 4, which exhibits the relative differences of moments together with the maximum particle amplitude at zero current. Since there are no space-charge forces, these differences are primarily due to the z-to-t transformation used before the moments are calculated and the finite time step size. For the reference case, the maximum value of the z-to-t transformation error, estimated from these figures, is about 0.1% through the system.

The accuracy of the z-to-t transformation in Eqs. (21)–(26) depends on the phase width or longitudinal length, the momentum spread, and the energy spread of the beam bunch. Increasing the current may deteriorate the accuracy of the transformation due to the increasing momentum and energy spread of the beam. Figure 5 shows the relative difference of the moments together with the maximum amplitude for a beam current of 400 mA in the reference case. In this case, the transverse tune depression is about 0.31, and the longitudinal tune depression is about 0.21. The maximum relative difference increases from 0.25% to 0.4%. The oscillation of the maximum transverse amplitude and the growth of the longitudinal amplitude, as seen in the figure, indicate that the beam is mismatched.

We have also investigated the dependence of the accuracy of the approximations on transverse and longitudinal focusing strength. In an rf linac design, the zero-current phase advance is generally kept below 90° to avoid beam envelope instabilities. Therefore, we examined two transverse cases, one with a transverse zero-current phase advance of 13°, the other with a phase advance of

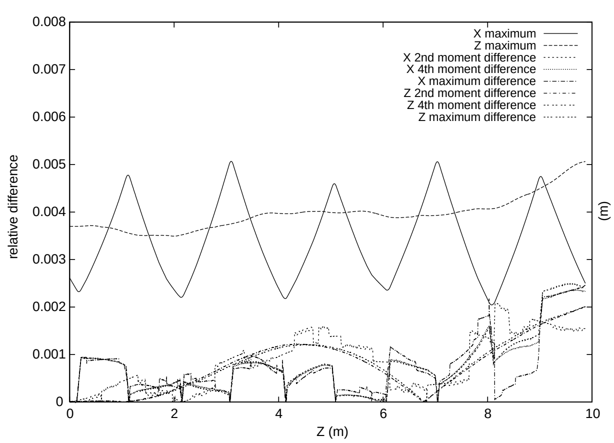

FIG. 3. The relative difference between the z-dependent macroparticle simulation and the t-dependent simulation, and the maximum particle amplitude as a function of position in the reference case.

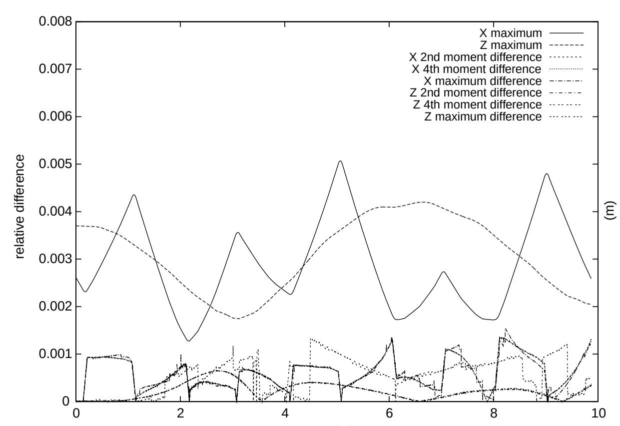

FIG. 4. The relative difference and maximum particle amplitude as a function of position using zero current in the reference case.

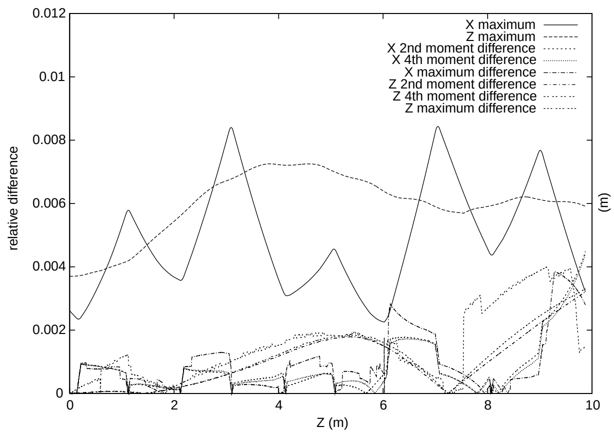

FIG. 5. The relative difference and maximum particle amplitude as a function of position using 400 mA current in the reference case.

90°. The relative differences between moments together with the particle maximum amplitude for these two cases, are given in Figs. 6a and 6b. We see that the maximum relative difference resulting from a weaker transverse focusing is about 0.7%, while the maximum relative difference due to a stronger transverse focusing is about 0.2%. The larger relative difference for the weaker focusing is due to transverse mismatch which causes beam blowup. This can be seen from the curves of X maximum and Z maximum in the figure. The effects of longitudinal focusing and acceleration were also investigated. We have made comparisons for zero-current longitudinal phase advance ranging from 18° to 79°. Figures 7a and 7b show the relative differences together with the maximum particle amplitudes for these two cases. We see that with longitudinal mismatch, the maximum longitudinal amplitude increases to more than 2.5 cm and the maximum relative difference is still only 0.2% as in the weaker focusing case. In the stronger focusing case, and with transverse mismatch, the maximum transverse amplitude is 7 mm, and the maximum relative difference is still only 0.3%. These results suggest that within the normal focusing regime, the maximum relative differences between the z-dependent macroparticle simulation and the t-dependent simulation are less than 1% for a strongly mismatched beam through a 10 m transport system. Comparing these results with the relative differences for the zero-current case, the maximum error contributed

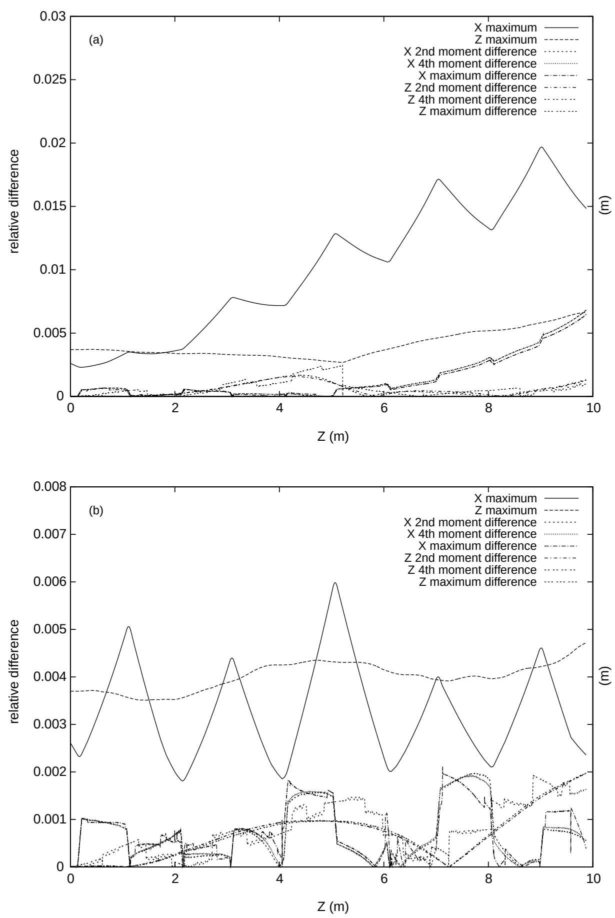

FIG. 6. The relative difference and maximum particle amplitude as a function of position for (a) weaker transverse focusing, and (b) stronger transverse focusing than the reference case.

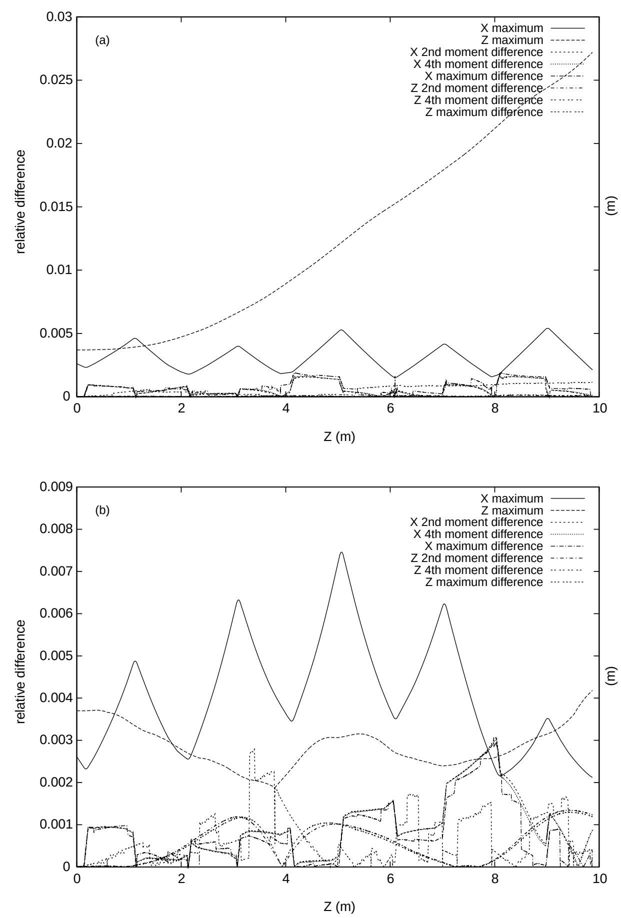

FIG. 7. The relative difference and maximum particle amplitude as a function of position for (a) weaker longitudinal focusing, and (b) stronger longitudinal focusing than the reference case.

by the z-to-t transformation for the space-charge force calculation is about 0.6% in the z-dependent simulation.

The initial emittance in the reference case is about 0.24 mm mrad transversely and longitudinally, and is similar to that of the SNS. Varying the emittance will affect the beam bunch size and momentum spread. This will also affect the accuracy of the z-to-t transformation for the calculation of the space-charge forces in the z-dependent simulation. Figure 8a shows the maximum particle amplitude for an initial distribution whose longitudinal rms size is 10 times larger than the initial bunch length of the reference case. This corresponds to a longitudinal emittance of 1.9 mm mrad. Figure 8b gives the transverse and longitudinal relative differences as a function of z for this case. We see that the maximum relative difference is about 0.4% with the mismatched maximum longitudinal amplitude as large as 25 cm. Figure 9 shows the relative moment differences and maximum amplitudes as a function of z for an initial distribution whose rms transverse momentum spread is 3 times the momentum spread in the reference case. The new initial transverse emittance is about 0.71 mm mrad. The maximum relative

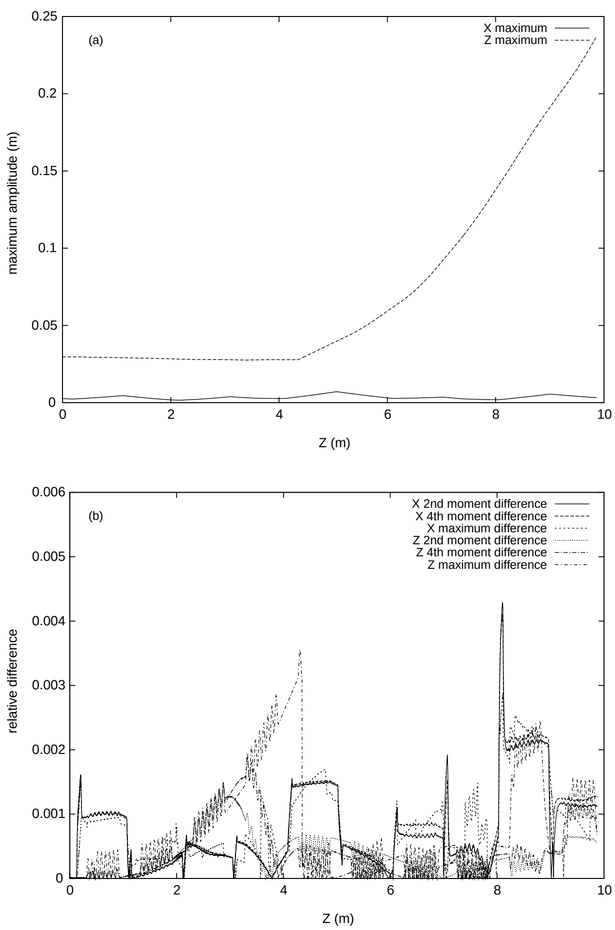

FIG. 8. (a) The maximum particle amplitude, (b) relative moment difference as a function of position with larger initial longitudinal emittance than the reference case.

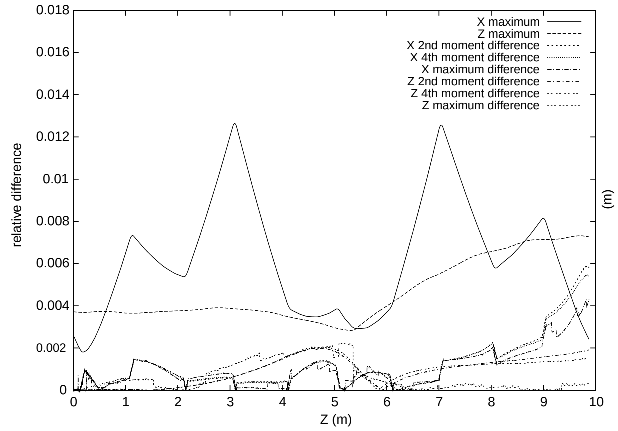

FIG. 9. The relative difference and maximum particle amplitude as a function of position with larger initial transverse emittance than the reference case.

difference is about 0.6% with a maximum mismatched amplitude of 1.3 cm.

At present, the zeroth-order transformation discussed earlier is used in the code PARMILA. Figure 10 gives the relative differences using the zeroth-order transformation in the reference case. We see that the maximum relative difference using the zeroth-order transformation is 0.25%. This is comparable to using the first-order transformation in the z-dependent simulation. However, in some severely mismatched cases, it appears that the maximum relative difference using the zeroth-order transformation can be much larger than that of using the first-order transformation. As an example of this, Fig. 11 gives the relative difference for the case of a larger longitudinal emittance and uses the zeroth-order transformation in the z-dependent simulation. Comparing this with Fig. 8b, we see that the maximum relative differences using the zeroth-order transformation are much larger than that of using the first-order transformation.

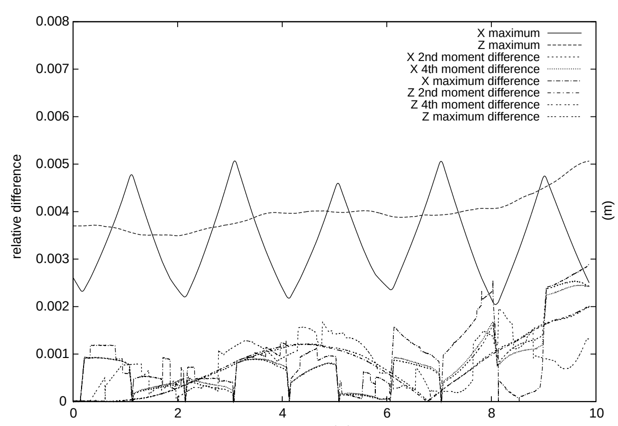

FIG. 10. The relative difference and maximum particle amplitude as a function of position using zeroth-order transformation in the reference case.

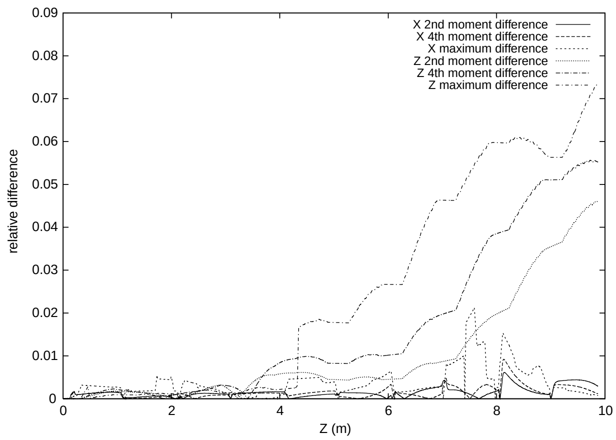

FIG. 11. The relative difference and maximum particle amplitude as a function of position using zeroth-order transformation with larger initial longitudinal emittance than the reference case.

The relative differences between moments could increase with increasing transport system length through an accumulation of errors. To see if this is true and to estimate the growth rates, we have repeated our simulations of the reference case with a transport length of 20 m. Figure 12 gives the relative differences together with the maximum amplitudes as a function of z. The large variation of the transverse and longitudinal maximum amplitudes after 10 m is due to a mismatch caused by a change in energy gain from 2 to 1 MeV/period after the first 10 m for fixed rf field amplitude. We see that the maximum relative difference increases from 0.25% in the first half of the transport system to 0.7% in the second half of the transport system. This growth results from large single-particle trajectories in the simulations. For the second and fourth moments, the maximum relative difference in the second section is about 0.3%. The maximum error in the space-charge calculation caused by the z-to-t transformation in the z code increases from 0.1% to 0.15% for the moments. It increases to 0.55% for the maximum transverse amplitude. By simple scaling, this suggests that for a linac that is several hundred meters long, the maximum errors caused only by the z-to-t transformation in a z-dependent simulation could be as large as several percent for the moments and up to approximately 10% for the maximum amplitude.

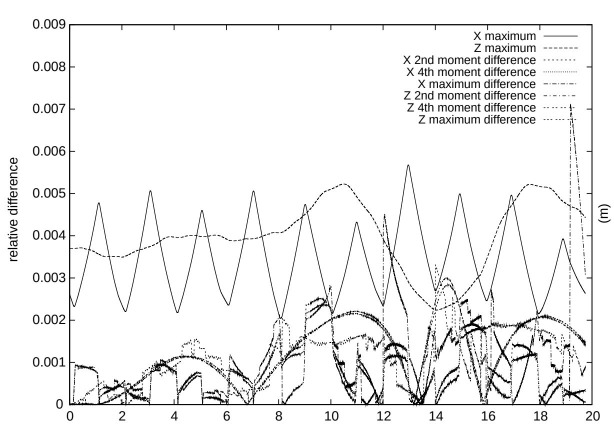

FIG. 12. The relative difference and maximum particle amplitude as a function of position with double-length reference transport system.

IV. CONCLUSIONS

In the above studies, we have calculated the relative moment differences between z-dependent macroparticle simulations and t-dependent macroparticle simulations under conditions of varying physical parameters. Several cases were examined with beam currents as high as 440 mA, zero-current transverse phase advances of 13° and 90°, longitudinal phase advances of 18° and 79°, transverse emittances up to 0.7 mm mrad, and longitudinal emittances up to 2 mm mrad. The maximum relative error of the z-to-t transformation for the calculation of space-charge forces in the z-dependent macroparticle simulation was found to be about 0.6% through a mismatched transport system of 10 m. These errors may be cumulative as the length of the transport system is increased and may be as high as 10%–20% when simulating a rf linac with a length of several hundred meters. We have assumed that by considering a mismatched beam we have examined cases which represent an upper boundary of the errors. In the better-matched reference case, the maximum error observed for transporting through the 10 m beam line is only about 0.1%. For a well-matched linac we expect only a few percent error. This small percentage discrepancy between the two codes is not expected to significantly improve the selection of parameters in a linac design. Other uncertainties in the design process such as the initial distribution, field and phase errors, misalignment errors, gas neutralization, wakefields, and other effects are expected to dominate. Based on our results, we feel that, for linac designs in the regime of the present study, it is justified to use z-dependent macroparticle simulations. However, caution is required in cases where a large accumulation of computational errors is to be avoided, such as in the study of charged-particle motion in a ring, where the integrated length of the transport system could be several to tens of thousands of meters as the particles move in the ring for many turns. In this situation, an error in the space-charge calculation due to the z-to-t transformation could be significant. Additionally, the example used in the current study assumed a 88 MeV kinetic energy for our input beam. Errors in the space-charge calculation due to the z-to-t transformation may be larger when the initial energy is lower or the bunch length is relatively longer, as may be the case for a beam in a DTL where the rf frequency has changed at injection and/or the accelerating field is being ramped. Our study has not addressed this regime. However, a recent study by Nath *et al.* describing simulation results for the first DTL tank of the SNS linac from 2.5 to 7.0 MeV suggests good agreement among codes using either z or t as the dependent variable [10]. In those situations, it may be necessary to use multiple reference trajectories to reduce the transformation error in the z-dependent macroparticle simulations. Finally, the above study suggests that the first-order transformation has smaller maximum errors as compared with the zeroth-order transformation and should be used in z-dependent simulations.

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